

# PRESERVATION OF STABILITY PROPERTIES NEAR FIXED POINTS OF LINEAR HAMILTONIAN SYSTEMS BY SYMPLECTIC INTEGRATORS

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ABSTRACT. Based on reasonable testing model problems, we study the preservation by symplectic Runge-Kutta method (SRK) and symplectic partitioned Runge-Kutta method (SPRK) of structures for fixed points of linear Hamiltonian systems. The structure-preservation region provides a practical criterion for choosing step-size in symplectic computation. Examples are given to justify the investigation.

## 1. INTRODUCTION AND PRELIMINARIES

Consider the  $n$ -degree-of-freedom (d.o.f) Hamiltonian system

$$(1.1) \quad \dot{\mathbf{z}} = J\nabla H(\mathbf{z}), \quad J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix},$$

where  $H$  is a smooth scalar function of the extended phase space variables  $\mathbf{z} \in \mathbb{R}^{2n}$ , denoting the Hamiltonian, and  $J$  is the Poisson matrix with  $I$  the  $n \times n$  identity matrix. By introducing the canonically conjugate variables,  $\mathbf{z} = (q, p)$ , the above system can be rewritten as

$$(1.2) \quad \dot{q} = \partial H / \partial p, \quad \dot{p} = -\partial H / \partial q,$$

where  $q \in \mathbb{R}^n$  represents the configuration coordinates of the system and their canonically conjugate momenta  $p \in \mathbb{R}^n$  represents the impetus gained by movement. As is well-known, Hamiltonian systems are introduced as a type of system for which the existence of conservative quantities are automatic. System (1.2) possesses two remarkable properties:

- (1) the solutions preserve the Hamiltonian, i.e.,

$$(1.3) \quad \frac{dH}{dt} = 0;$$

- (2) the corresponding flow is symplectic, i.e.,

$$(1.4) \quad \frac{d}{dt}[dp \wedge dq] = 0.$$

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In the last two decades, enormous attention has been paid to numerical methods which preserve the symplecticity, namely, symplectic integrators for Hamiltonian systems; we refer to the monographs Hairer *et al.* [1] and Sanz-Serna&Calvo [8] for details and related literature. Theoretical analysis together with numerous numerical experiments has shown that symplectic integrator not only produces improved qualitative numerical behaviors, but also allows for a more accurate long-time scale computation than with general-purpose methods. In the symplectic integration study, a widely recognized fact is that the symplecticity of a numerical integrator has little to do with its step-size. Particularly, for SRK and SPRK methods, their symplecticities are only related to the coefficients (see Section 2 below). Therefore, in practical computations, one usually resorts to the classical stability analyses to find a suitable range for choosing numerical step-sizes. However, in a recent paper [3], it is shown that in some cases even the step-size of the symplectic Euler method satisfies the classical linear stability requirements, one can still get periodic-two numerical solutions, or even chaotic solutions. That means, we need to require more stringent conditions on step-sizes in addition to the classical stability considerations in simulations of Hamiltonian flows, even for symplectic integrators. In the present paper, we make a first step towards such investigation by studying the influence induced by the numerical discretization on the equilibria structure of the underlying Hamiltonian system. It is recalled that for a general ODE of the form

$$\dot{\mathbf{z}} = f(\mathbf{z}), \quad \mathbf{z} \in \mathbb{R}^m, \quad f: \mathbb{R}^m \mapsto \mathbb{R}^m,$$

it may admit the presence of equilibrium point, namely,  $\tilde{\mathbf{z}} \in \mathbb{R}^m$  such that  $f(\tilde{\mathbf{z}}) = 0$ , and the eigenvalues of the corresponding stability matrix  $\nabla_{\mathbf{z}}f(\tilde{\mathbf{z}})$  determine the type of the equilibrium point and its stability properties.

In the sequel, we are mainly concerned with the Runge-Kutta (RK) methods and partitioned Runge-Kutta (PRK) methods. Henceforth, we customarily refer to an  $s$ -stage RK method by the triple  $\mathcal{R}_s = (A, b, c)$ , with  $A = (a_{ij})_{i,j=1}^s$ ,  $b = (b_i)_{i=1}^s$  and  $c = (c_i)_{i=1}^s$  being, respectively, the coefficient matrix, weights and abscissae, and an  $s$ -stage PRK method by the pair  $\mathcal{R}_s^{(1)} - \mathcal{R}_s^{(2)}$ . Next, we would like to review some of the classical linear stability concepts and by tracing the origins we can thus draw forth our motivations for the current work. The probably most well known A-stability is introduced by Dahlquist in 1960's (see, e.g., [2]). Applying  $\mathcal{R}_s$  to the famous Dahlquist test equation

$$(1.5) \quad y' = \lambda y, \quad \lambda \in \mathbb{C}, \quad \Re \lambda < 0,$$

we get the following scheme

$$(1.6) \quad y_{l+1} = R(z)y_l, \quad l = 0, 1, 2, \dots, \quad \text{and} \quad z = \lambda h,$$

with  $R(z)$  the stability function of  $\mathcal{R}_s$  (see, Chapter IV.3, [2]). It is noted that the solution to (1.5) asymptotically decays to zero as  $t \rightarrow \infty$ , and in order for the numerical scheme (1.6) to yield such qualitative behavior

without any restriction on the step size  $h$ , we naturally require that

$$(1.7) \quad |R(z)| < 1, \quad \text{for any } h > 0.$$

Methods satisfying (1.7) are called A-stable, and this concept has been playing an indispensable role in the numerical field. Apparently, one can derive the same conclusion (1.7) for  $\mathcal{R}_s$  when applying it to the following equation

$$(1.8) \quad y' = \bar{\lambda}y,$$

where  $\bar{\lambda} \in \mathbb{C}$  is the complex conjugate to  $\lambda$  in equation (1.5). If we set  $\lambda = \alpha + i\beta$  with  $\alpha, \beta \in \mathbb{R}$  and  $\alpha < 0$ , it is easy to see that equations (1.5) and (1.8) are equivalent to the following system of ODE,

$$(1.9) \quad \begin{cases} \dot{x} = \alpha x - \beta y, \\ \dot{y} = \beta x + \alpha y. \end{cases}$$

System (1.9) has an equilibrium point  $(0, 0)$  and its corresponding stability matrix is given by

$$\mathbf{J} = \begin{bmatrix} \alpha & -\beta \\ \beta & \alpha \end{bmatrix},$$

which has two eigenvalues  $\lambda_{1,2} = \alpha \pm i\beta$ . Now, we apply  $\mathcal{R}_s$  to (1.9) and get

$$(1.10) \quad \begin{bmatrix} x_{l+1} \\ y_{l+1} \end{bmatrix} = Q \begin{bmatrix} R(z) & 0 \\ 0 & R(\bar{z}) \end{bmatrix} Q^{-1} \begin{bmatrix} x_l \\ y_l \end{bmatrix}$$

with

$$z = \lambda h, \quad \bar{z} = \bar{\lambda}h, \quad \lambda = \alpha + i\beta \quad \text{and} \quad Q = \frac{1}{\sqrt{2}} \begin{bmatrix} i & -1 \\ 1 & -i \end{bmatrix}.$$

Introducing the forward difference operators

$$\delta_t^+ x_l = \frac{x_{l+1} - x_l}{h}, \quad \delta_t^+ y_l = \frac{y_{l+1} - y_l}{h},$$

scheme (1.10) can be reformulated into

$$(1.11) \quad \delta_t^+ \begin{bmatrix} x_l \\ y_l \end{bmatrix} = Q \begin{bmatrix} \frac{R(z)-1}{h} & 0 \\ 0 & \frac{R(\bar{z})-1}{h} \end{bmatrix} Q^{-1} \begin{bmatrix} x_l \\ y_l \end{bmatrix},$$

which is the discrete dynamical system approximating (1.9). Obviously,  $(0, 0)$  is the fixed point (equilibrium point) for (1.11) and the corresponding stability matrix is given by the coefficient matrix in (1.11), which is seen to possess two eigenvalues,  $\lambda_{h,1} = (R(z) - 1)/h$ ,  $\lambda_{h,2} = \bar{\lambda}_{h,1}$ . Now, it is readily seen that an A-stable RK method preserves the equilibria structure unconditionally after discretization. In the reverse, if we want an RK method to give rise to certain preservation of the equilibria structure of the underlying ODE, we are naturally led to the condition (1.7). From above analyses, we can further easily deduce that the so-called stability region for an RK method (see, Chapter IV.3, [2]) is indeed the set of those step sizes with which the RK method can preserve the equilibria structure of the test equation (1.9).

Next, we briefly mention one more example to illustrate the close connection between the so-called P-stability and the preservation of equilibria structure. In the theory of orbital mechanics, many problems are formulated as some special second order ODE

$$(1.12) \quad \frac{d^2 u}{dt^2} = f(t, u), \quad u(t_0) = u_0, \quad \dot{u}(t_0) = u'_0,$$

which is often known in advance to have periodic solution. In [4], Lambert and Watson introduced the concept of P-stability for numerical methods to solve equation (1.12). It is remarked that in [4], the P-stability is defined for multistep methods, while it is equally applicable to RK method. The test model problem given in [4] is

$$(1.13) \quad \ddot{u} = -\lambda^2 u, \quad \lambda \in \mathbb{R}.$$

Set  $\dot{u} = v$ , then equation (1.13) can be reformulated into a first order system

$$(1.14) \quad \begin{cases} \dot{u} = v, \\ \dot{v} = -\lambda^2 u. \end{cases}$$

In like manner as above for A-stability, one can show that the P-stable RK methods for (1.13) preserve the equilibria structure of (1.14) unconditionally and vice versa. However, we will not explore more details on this aspect and now turn our study to Hamiltonian system (1.1).

The equilibrium points of system (1.1) are those  $(\tilde{p}, \tilde{q}) \in \mathbb{R}^n \times \mathbb{R}^n$  such that  $\nabla H(\tilde{p}, \tilde{q}) = 0$  and the corresponding stability matrices are given by

$$\mathbf{J}_S(\tilde{p}, \tilde{q}) := \frac{\partial(-\partial H/\partial q, \partial H/\partial p)}{\partial(p, q)}(\tilde{p}, \tilde{q}).$$

To ease our study, we start with linear Hamiltonian systems, and then propose several ways to extend our analyses to nonlinear case. We first designate some model problems for our investigation. Apparently, these model problems should feature the Hamiltonian systems. In [7], it is shown that an  $n$  d.o.f linear Hamiltonian system can be canonically transformed into a Hamiltonian system consisting of  $n$  1-d.o.f subsystems and these subsystems assume the following standard forms,

$$(1.15) \quad \begin{cases} \dot{p} = -\beta^2 q, \\ \dot{q} = p, \end{cases} \quad \beta > 0$$

or

$$(1.16) \quad \begin{cases} \dot{p} = -\beta p, \\ \dot{q} = \beta q, \end{cases} \quad \beta > 0.$$

Therefore, it is natural for us to take systems (1.15) and (1.16) as our testing model problems and which will be used throughout. Clearly,  $(0, 0)$  is their

equilibrium point, and for system (1.15)

$$\mathbf{J}_s = \begin{bmatrix} 0 & -\beta^2 \\ 1 & 0 \end{bmatrix}$$

with corresponding eigenvalues  $\lambda_{1,2} = \pm i\beta$ , which are of elliptic type, and we call system (1.15) have elliptic equilibria structure; while for system (1.16)

$$\mathbf{J}_s = \begin{bmatrix} -\beta & 0 \\ 0 & \beta \end{bmatrix}$$

with the eigenvalues  $\lambda_{1,2} = \pm\beta$ , which are of hyperbolic type, and we call system (1.16) having hyperbolic equilibria structure. Next, we shall investigate under what conditions, the equilibria structure can be inherited by the corresponding numerical schemes. And what would be caused by the numerical discretization if the structure-preservation conditions are ruined.

In the section followed, we present some necessary and sufficient conditions for an SRK/SPRK method and its corresponding symmetric composition method to preserve the equilibria structures of the testing problems. The fundamental idea is that we regard the numerical scheme as a discrete dynamic which is an approximation to the Hamiltonian system and therefore should have the same equilibria structure as its continuous counterpart. Results show that in some cases, SRK method can preserve the equilibria structure unconditionally, but without exception, PRK method always gives a structure-preservation region on the positive real line for the numerical step-size. Furthermore, it is found that if the order of accuracy of a SPRK method is increased by symmetric composition, the structure-preservation region will be decreased accordingly.

In section 3, we extend the analyses to nonlinear Hamiltonian systems. Besides, we give an example which justifies the necessities of such equilibria structure preservation study.

## 2. EQUILIBRIA STRUCTURE PRESERVATION OF SRK/SPRK METHOD

In this paper, we confine our study to symplectic Runge-Kutta (SRK) methods and symplectic partitioned Runge-Kutta (SPRK) methods. The symplecticity conditions for  $\mathcal{R}_s$  and  $\mathcal{R}_s^{(1)} - \mathcal{R}_s^{(2)}$  are, respectively, given by (see [1],[8])

$$(2.1) \quad BA + A^T B - bb^T = 0, \quad B = \text{diag}[b];$$

$$(2.2) \quad B^{(2)}A^{(1)} + A^{(2)T}B^{(1)} - b^{(2)}b^{(1)T} = 0, \quad B^{(i)} = \text{diag}[b^{(i)}] \quad (i = 1, 2),$$

$$(2.3) \quad b^{(1)} = b^{(2)}.$$

**2.1. Preserving the elliptic equilibria structure.** We first apply  $\mathcal{R}_s$  to system (1.15) and get the following scheme

$$(2.4) \quad \begin{cases} P = p_l e_s - h\beta^2 A Q, & p_{l+1} = p_l - h\beta^2 b^T Q, \\ Q = q_l e_s + h A P, & q_{l+1} = q_l + h b^T P, \end{cases}$$

where  $P = [P_1, P_2, \dots, P_s]^T$  and  $Q = [Q_1, Q_2, \dots, Q_s]^T$  are internal stage values,  $e_s = [1, \dots, 1]^T$  and  $p_l \approx p(lh), q_l \approx q(lh)$ . It can be computed straightforwardly that

$$\begin{cases} P = (I + h^2\beta^2 A^2)^{-1}(e_s p_l - h\beta^2 A e_s q_l), \\ Q = (I + h^2\beta^2 A^2)^{-1}(e_s q_l + hA e_s p_l), \end{cases}$$

and thus scheme (2.4) is equivalently reformulated as

$$(2.5) \quad \begin{cases} \delta_t^+ p_l = -h\beta^2 D A e_s p_l - \beta^2 D e_s q_l, \\ \delta_t^+ q_l = D e_s p_l - h\beta^2 D A e_s q_l, \end{cases}$$

where  $D = b^T(I + h^2\beta^2 A^2)^{-1}$  and the forward difference operators are defined as

$$\delta_t^+ p_l = \frac{p_{l+1} - p_l}{h}, \quad \delta_t^+ q_l = \frac{q_{l+1} - q_l}{h}.$$

(2.5) is a discrete dynamical system which approximates (1.15) and obviously,  $(0, 0)$  is its fixed point (equilibrium point). The stability matrix of (2.5) is

$$\mathbf{J}_N = \begin{bmatrix} -h\beta^2 D A e_s & -\beta^2 D e_s \\ D e_s & -h\beta^2 D A e_s \end{bmatrix}$$

and its eigenvalues are

$$\tilde{\lambda}_{1,2} = -h\beta^2 D A e_s \pm i(\beta D e_s),$$

which are of elliptic type. Hence, the SRK method preserves the elliptic equilibria structure of system (1.15) unconditionally, but here we note that there is a little shift of  $\tilde{\lambda}_{1,2}$  from  $\lambda_{1,2}$  due to the numerical discretization. Next, we apply an  $s$ -stage SPRK method  $\mathcal{R}_s^{(1)} - \mathcal{R}_s^{(2)}$  to system (1.15) and get the following scheme

$$(2.6) \quad \begin{cases} P = p_l e_s - h\beta^2 A^{(1)} Q, & p_{l+1} = p_l - h\beta^2 b^{(1)T} Q, \\ Q = q_l e_s + hA^{(2)} P, & q_{l+1} = q_l + h b^{(2)T} P. \end{cases}$$

The discrete dynamical system equivalent to (2.6) is given by

$$(2.7) \quad \begin{cases} \delta_t^+ p_l = -h\beta^2 D^{(1)} A^{(2)} e_s p_l - \beta^2 D^{(1)} e_s q_l, \\ \delta_t^+ q_l = D^{(2)} e_s p_l - h\beta^2 D^{(2)} A^{(1)} e_s q_l, \end{cases}$$

where

$$(2.8) \quad D^{(1)} = b^{(1)T}(I + h^2\beta^2 A^{(2)} A^{(1)})^{-1}, \quad D^{(2)} = b^{(2)T}(I + h^2\beta^2 A^{(1)} A^{(2)})^{-1}.$$

The stability matrix for (2.7) is

$$\mathbf{J}_N = \begin{bmatrix} -h\beta^2 D^{(1)} A^{(2)} e_s & -\beta^2 D^{(1)} e_s \\ D^{(2)} e_s & -h\beta^2 D^{(2)} A^{(1)} e_s \end{bmatrix},$$

and its eigenvalues are

$$\begin{aligned} \tilde{\lambda}_{1,2} = & \frac{1}{2} \left\{ -h\beta^2 [D^{(1)}A^{(2)}e_s + D^{(1)}A^{(2)}e_s] \right. \\ & \left. \pm \sqrt{h^2\beta^4 [D^{(1)}A^{(2)}e_s - D^{(2)}A^{(1)}e_s]^2 - 4\beta^2 [(D^{(1)}e_s)(D^{(2)}e_s)]} \right\}. \end{aligned}$$

Therefore, if the equilibria point  $(0, 0)$  for (2.7) is of elliptic type we need to require

$$(2.9) \quad h^2\beta^2 [D^{(1)}A^{(2)}e_s - D^{(2)}A^{(1)}e_s]^2 - 4[(D^{(1)}e_s)(D^{(2)}e_s)] < 0.$$

Next, we introduce

$$(2.10) \quad \begin{aligned} a_1 &:= \frac{\det(I + z^2 A^{(2)}(A^{(1)} - e_s b^{(1)T}))}{\det(I + z^2 A^{(2)}A^{(1)})}, \\ a_2 &:= \frac{\det(I + z^2 A^{(1)}(A^{(2)} - e_s b^{(2)T}))}{\det(I + z^2 A^{(1)}A^{(2)})}, \end{aligned}$$

where  $z = \beta h$ , which shall also be used throughout, then condition (2.9) can be reformulated as

$$(2.11) \quad |a_1 + a_2| < 2.$$

In fact, from (2.7), one can get

$$(2.12) \quad \begin{aligned} p_{l+1} &= (1 - z^2 D^{(1)}A^{(2)}e_s)p_l - \beta z D^{(1)}e_s q_l, \\ q_{l+1} &= h D^{(2)}e_s p_l + (1 - z^2 D^{(2)}A^{(1)}e_s)q_l. \end{aligned}$$

Since the method is symplectic, it has

$$dp_{l+1} \wedge dq_{l+1} = dp_l \wedge dq_l.$$

Substituting the relations (2.12) into the above equality, then through straightforward calculations, we obtain

$$(D^{(1)}e_s)(D^{(2)}e_s) = [D^{(1)}A^{(2)}e_s + D^{(2)}A^{(1)}e_s] - z^2(D^{(1)}A^{(2)}e_s)(D^{(2)}A^{(1)}e_s),$$

which is then substituted into (2.9) to yield

$$(2.13) \quad |1 - z^2 D^{(1)}A^{(2)}e_s + 1 - z^2 D^{(2)}A^{(1)}e_s| < 2.$$

Next, by observing that

$$\begin{aligned} 1 - z^2 D^{(1)}A^{(2)}e_s &= 1 - z^2 b^{(1)T} (I + h^2 \beta^2 A^{(2)}A^{(1)})^{-1} A^{(2)}e_s = a_1, \\ 1 - z^2 D^{(2)}A^{(1)}e_s &= 1 - z^2 b^{(2)T} (I + h^2 \beta^2 A^{(1)}A^{(2)})^{-1} A^{(1)}e_s = a_2, \end{aligned}$$

we finally arrive at the equivalence of (2.9) and (2.11)

In summary, we have

**Proposition 2.1.** *For system (1.15), an SRK method  $\mathcal{R}_s$  preserves its elliptic equilibria structure unconditionally, whereas for an SPRK method,  $\mathcal{R}_s^{(1)} - \mathcal{R}_s^{(2)}$ , its structure-preservation region is given by*

$$(2.14) \quad \{h > 0 : |a_1 + a_2| < 2\},$$

where  $a_1$  and  $a_2$  are defined by (2.10).

Consider the symplectic Euler method, where  $A^{(1)} = 0, A^{(2)} = 1$  and  $b^{(1)} = b^{(2)} = 1$ . By (2.10), it is computed that  $a_1 = 1 - z^2, a_2 = 1$ , and hence for symplectic Euler method to preserve the elliptic structure of system (1.15) we must have from (2.14) that  $|2 - z^2| < 2$ , i.e.,  $0 < \beta h < 2$ .

Using the W-transformation due to Hairer and Wanner (see Chapter IV.5, [2]), we have

$$(2.15) \quad W^{-1}A^{(1)}W = X_{A^{(1)}}, \quad W^{-1}A^{(2)}W = X_{A^{(2)}},$$

where  $W$  is the generalized Vandermonde matrix, and  $X_{A^{(i)}} (i = 1, 2)$  are matrices possessing some standard form. In particular, for a class of important symplectic method, Lobatto IIIA-Lobatto IIIB pair (see [9, 10]),

$$(2.16) \quad X_{A^{(1)}} = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & & \\ \xi_1 & 0 & \ddots & & \\ & \ddots & \ddots & -\xi_{s-2} & \\ & & \xi_{s-2} & 0 & 0 \\ & & & \xi_{s-1} & 0 \end{pmatrix},$$

$$(2.17) \quad X_{A^{(2)}} = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & & \\ \xi_1 & 0 & \ddots & & \\ & \ddots & \ddots & -\xi_{s-2} & \\ & & \xi_{s-2} & 0 & -\xi_{s-1} \\ & & & 0 & 0 \end{pmatrix},$$

where  $\xi_k = 1/2\sqrt{4k^2 - 1}, k = 1, 2, \dots, s$ . In term of W-transformation, i.e., using (2.15),  $a_i (i = 1, 2)$  in (2.10) can be reformulated as

$$(2.18) \quad a_1 = \frac{\det(I + z^2 X_{A^{(2)}}(X_{A^{(1)}} - e^1 e^{1T}))}{\det(I + z^2 X_{A^{(2)}} X_{A^{(1)}})},$$

$$(2.19) \quad a_2 = \frac{\det(I + z^2 X_{A^{(1)}}(X_{A^{(2)}} - e^1 e^{1T}))}{\det(I + z^2 X_{A^{(1)}} X_{A^{(2)}})},$$

where  $e^1 = [1, 0, \dots, 0, 1]^T$ . For Lobatto IIIA-Lobatto IIIB pair, with  $X_{A^{(i)}} (i = 1, 2)$  given in (2.16) and (2.17), it is easily verified that  $a_1 = a_2$  and therefore, for Lobatto IIIA-Lobatto IIIB method to preserve the elliptic structure of system (1.15) we must have from (2.14) that  $|a_1| < 1$ . In the following, we list some of the computed results for Lobatto IIIA-Lobatto IIIB method in term of its stage  $s$ ; see Table 1. Moreover, for  $s = 5$ , the structure-preservation region is  $0 < z < 3.140328$ , and for  $s = 10$ , it is



TABLE 1. Structure-preservation region for Lobatto IIIA-Lobatto IIIB pair

$s$	$a_1$	$z$
2	$1 - \frac{1}{2}z^2$	$0 < z < 2$
3	$\frac{1 - \frac{11}{24}z^2 + \frac{1}{48}z^4}{1 + \frac{1}{24}z^2}$	$0 < z < \sqrt{8}(\approx 2.828)$
4	$\frac{1 - \frac{7}{15}z^2 + \frac{23}{900}z^4 - \frac{1}{3600}z^6}{1 + \frac{1}{30}z^2 + \frac{1}{1800}z^4}$	$0 < z < \sqrt{42 - 6\sqrt{29}}(\approx 3.1127)$

$0 < z < 3.141590$ . We are naturally led to the conjecture that as  $s \rightarrow \infty$ , the elliptic structure-preservation region for an  $s$ -stage Lobatto IIIA-Lobatto IIIB method is given by  $0 < z < \pi$ .

Next, we consider the composition of a given basic one-step method with different step sizes,

$$(2.20) \quad \Psi_h = \Phi_{\gamma_s h} \circ \cdots \circ \Phi_{\gamma_1 h},$$

where  $\Phi_h$  is the basic SRK method and  $\gamma_i h (i = 1, \dots, s)$  are the composition step length (cf. [6],[11]). The composition is required to be symmetric, i.e.,  $\gamma_i = \gamma_{s+1-i} (i = 1, 2, \dots, [s/2])$ , and hence  $\Psi_h$  is still an SRK method. By Proposition 2.1, we know that the symmetric composition of an SRK method still preserves the elliptic structure of system (1.15) unconditionally. Next, consider the structure-preservation region of a symmetric composition of a SPRK method, which is known to be again a SPRK method. To ease our study, we only take the 2-stage Lobatto IIIA-Lobatto IIIB pair as an example, whose 4th-order symmetric composition is given in [5], and for which we compute

$$a_1 = 1 - \frac{1}{2}z^2 + \frac{1}{4}\gamma_1^2\gamma_2^2(5\gamma_1 + 4\gamma_2)z^4 - \frac{1}{8}\gamma_1^3\gamma_2(\gamma_1 + \gamma_2)^2z^6,$$

where  $\gamma_1 = 1/(2 - 2^{1/3})$  and  $\gamma_2 = 2^{1/3}/(2 - 2^{1/3})$ . By  $|a_1| < 1$ , we get

$$0 < z < \sqrt{2.48}(\approx 1.5748).$$

Similarly, we further computed that the structure-preservation region for the corresponding 6th-order composition method is given by  $0 < z < 1.1034$ . Noting by Table 1, the structure-preservation region for the underlying basic method is  $0 < z < 2$ . Base on this example, we conjecture that as the order of a SPRK method is increased by symmetric composition, its structure-preservation region will be decreased accordingly. A stringent proof of such conjecture is fraught with difficulties and is beyond the scope of this paper.

**2.2. Preserving the hyperbolic equilibria structure.** The scheme of an SRK method  $\mathcal{R}_s$  for system (1.16) is read as

$$(2.21) \quad \begin{cases} \delta_t^+ p_l = \frac{R(-z)-1}{h} p_l, \\ \delta_t^+ q_l = \frac{R(z)-1}{h} q_l, \end{cases}$$

where  $R(z) = \det(I + zA)/\det(I - zA)$  is the stability matrix for  $\mathcal{R}_s$ . It is readily observed that for the discrete dynamical system (2.21) to preserve the equilibria structure of system (1.16), we must have

$$(2.22) \quad R(-z) - 1 < 0, \quad \text{and} \quad R(z) - 1 > 0,$$

i.e., the hyperbolic structure-preservation region for an SRK method  $\mathcal{R}_s$  is

$$(2.23) \quad \{h > 0 : \frac{\det(I - zA)}{\det(I + zA)} < 1 \text{ and } \frac{\det(I + zA)}{\det(I - zA)} > 1, z = \beta h\}.$$

Since we always have  $R(-z) < 1 (z = \beta h > 0)$  for an A-stable RK method. Hence, if the RK method  $\mathcal{R}_s$  is A-stable, in order to preserve the hyperbolic structure, we only need to require

$$(2.24) \quad \frac{\det(I + zA)}{\det(I - zA)} > 1.$$

Now, we show that the above inequality can be equivalently reduced to

$$(2.25) \quad \det(I - zA) > 0.$$

Indeed, since  $\mathcal{R}_s$  is A-stable, the eigenvalues of its coefficient matrix must lie on the right half plane, which implies  $\det(I + zA) > 0$  for  $z > 0$ , and this together with (2.24) further implies that  $\det(I - zA) > 0$ . Next, using again the fact that the eigenvalues of  $A$  lie on the right half plane, we have that

$$\frac{\det(I + zA)}{\det(I - zA)} > 1,$$

if  $z > 0$  satisfying  $\det(I - zA) > 0$ . Therefore, the hyperbolic equilibria structure-preservation region of an A-stable SRK method  $\mathcal{R}_s$  is given by

$$(2.26) \quad \{h > 0 : \det(I - zA) > 0, z = \beta h\}.$$

For example, the hyperbolic structure-preservation region for the well-known midpoint formula, where  $A = 1/2$  is given by

$$(2.27) \quad \{h > 0 : 1 - \frac{1}{2}\beta h > 0\} = \{h > 0 : \beta h < 2\}.$$

It is readily seen that even for SRK method which possesses good classical stability properties, we should still require some restrictions on its step-sizes for practical computations. Therefore, the investigations on the equilibria structure preservation provide a novel and useful criteria to choose step-sizes for symplectic integrators in addition to the classical linear stability requirements.

We now apply an  $s$ -stage SPRK method  $\mathcal{R}_s^{(1)} - \mathcal{R}_s^{(2)}$  to system (1.16) and get the following scheme

$$(2.28) \quad \begin{cases} \delta_t^+ p_l = \frac{R^{(1)}(-z)-1}{h} p_l, \\ \delta_t^+ q_l = \frac{R^{(2)}(z)-1}{h} q_l, \end{cases}$$

where  $R^{(i)}(z) = \det(I - zA^{(i)} + ze_s b^{(i)T}) / \det(I - zA^{(i)})$  ( $i = 1, 2$ ), are the stability matrices for  $\mathcal{R}_s^{(i)}$  ( $i = 1, 2$ ). Consequently, the hyperbolic structure-preservation region for  $\mathcal{R}_s^{(1)} - \mathcal{R}_s^{(2)}$  is

$$(2.29) \quad \{h > 0 : R^{(1)}(-z) < 1 \text{ and } R^{(2)}(z) > 1, z = \beta h\}.$$

For the well-known Lobatto IIIA-Lobatto IIIB pair,  $\mathcal{R}_s^{(1)} - \mathcal{R}_s^{(2)}$ , since both Lobatto IIIA method ( $\mathcal{R}_s^{(1)}$ ) and Lobatto IIIB method ( $\mathcal{R}_s^{(2)}$ ) are symmetric A-stable RK method, and therefore  $R^{(i)}(z) = \det(I + zA^{(i)}) / \det(I - zA^{(i)})$  ( $i = 1, 2$ ). Similar to (2.26), condition (2.29) is reduced to

$$(2.30) \quad \{h > 0 : \det(I - zA^{(i)}) > 0, i = 1, 2, z = \beta h\}.$$

for Lobatto IIIA-Lobatto IIIB method, where in particular, we note that  $\det(I - zA^{(i)}) = \det(I - zX_{A^{(i)}}) = \det(I - zX_{A^{(2)}})$  ( $i = 1, 2$ ) with  $X_{A^{(i)}}$  ( $i = 1, 2$ ) given in (2.16) and (2.17).

In summary, we have

**Proposition 2.2.** *The hyperbolic equilibria structure-preservation region of an SRK method  $\mathcal{R}_s$  for system (1.16) is*

$$\{h > 0 : \frac{\det(I - zA)}{\det(I + zA)} < 1 \text{ and } \frac{\det(I + zA)}{\det(I - zA)} > 1, z = \beta h\},$$

and this condition is reduced to

$$\{h > 0 : \det(I - zA) > 0, z = \beta h\},$$

if  $\mathcal{R}_s$  is A-stable. For an SPRK method,  $\mathcal{R}_s^{(1)} - \mathcal{R}_s^{(2)}$ , the hyperbolic structure-preservation region is given by

$$\{h > 0 : R^{(1)}(-z) < 1 \text{ and } R^{(2)}(z) > 1, z = \beta h\},$$

where  $R^{(1)}$  and  $R^{(2)}$  are, respectively, the stability functions for  $\mathcal{R}_s^{(1)}$  and  $\mathcal{R}_s^{(2)}$ .

Now, we consider the structure-preservation of the symmetric composition method (2.20). The 4th order symmetric composition of mid-point formula for system (1.16) is

$$(2.31) \quad \begin{cases} p_{l+1} = \frac{(1 - \gamma_1 z)(1 - \gamma_2 z)(1 - \gamma_3 z)}{(1 + \gamma_1 z)(1 + \gamma_2 z)(1 + \gamma_3 z)} p_l, \\ q_{l+1} = \frac{(1 + \gamma_1 z)(1 + \gamma_2 z)(1 + \gamma_3 z)}{(1 - \gamma_1 z)(1 - \gamma_2 z)(1 - \gamma_3 z)} q_l \end{cases}$$

with  $z = \beta h$ ,  $\gamma_1 = 1/(2 - 2^{1/3})$  and  $\gamma_2 = 2^{1/3}/(2 - 2^{1/3})$ . Therefore, for scheme to preserve the hyperbolic structure, we have

$$1 - \frac{z}{2 - 2^{1/3}} > 0 \quad \text{and} \quad 1 - \frac{2^{1/3}z}{2 - 2^{1/3}} > 0,$$

which yields

$$(2.32) \quad 0 < z < \frac{2 - 2^{1/3}}{2^{1/3}} (\approx 0.587401).$$

Clearly, in comparison with (2.27), the structure-preservation region becomes smaller after composing. This result applies equally to the SPRK method. Consider the following symplectic Euler method for system (1.16),

$$(2.33) \quad \begin{cases} p_{l+1} = (1 - z)p_l, \\ q_{l+1} = \frac{1}{1 - z}q_l, \end{cases} \quad z = \beta h,$$

whose structure-preservation region can be verified to be

$$(2.34) \quad 0 < z < 1.$$

Since the 2nd order symmetric composition of symplectic Euler method is the midpoint formula, hence the structure-preservation region of the 4th order symmetric composition of scheme (2.33) is given by (2.32), which is obviously decreased in comparison with (2.34).

### 3. EXTENSIONS TO NONLINEAR HAMILTONIAN SYSTEMS AND SOME APPLICATIONS

In this section, we extend the analyses in the previous sections to the nonlinear 1-d.o.f. Hamiltonian system

$$(3.1) \quad \begin{cases} \dot{p} = -\partial H / \partial q := f(p, q), \\ \dot{q} = \partial H / \partial p := g(p, q), \end{cases}$$

with  $(p, q) \in \mathbb{R}^2$ . We denote by  $\mathcal{E}_H$  the set of equilibrium points for system (3.1), i.e.,

$$\mathcal{E}_H := \left\{ (\tilde{p}, \tilde{q}) \in \mathbb{R}^2; \nabla_{(p,q)} H(\tilde{p}, \tilde{q}) = 0 \right\}.$$

The stability matrix for system (3.1) is locally defined for every  $(\tilde{p}, \tilde{q}) \in \mathcal{E}_H$  as

$$(3.2) \quad \mathbf{J}_S(\tilde{p}, \tilde{q}) = \begin{bmatrix} \partial f / \partial p & \partial f / \partial q \\ \partial g / \partial p & \partial g / \partial q \end{bmatrix} (\tilde{p}, \tilde{q}),$$

whose eigenvalues are given by

$$\lambda_{1,2} = \pm \sqrt{D}$$

with

$$D := D(\tilde{p}, \tilde{q}) = \left[ \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} - \frac{\partial f}{\partial p} \frac{\partial g}{\partial q} \right] (\tilde{p}, \tilde{q}).$$

Therefore, we can make the following classification:

- (i) If  $D(\tilde{p}, \tilde{q}) < 0$  for all  $(\tilde{p}, \tilde{q}) \in \mathcal{E}_H$ , then the equilibrium points for system (3.1) are all of elliptic type, and we then call system (3.1) having elliptic equilibria structure;

- (ii) If  $D(\tilde{p}, \tilde{q}) > 0$  for all  $(\tilde{p}, \tilde{q}) \in \mathcal{E}_H$ , then the equilibrium points for system (3.1) are all of hyperbolic type, and we call system (3.1) having hyperbolic equilibria structure;
- (iii) If  $D(\tilde{p}, \tilde{q}) \geq 0$  for some  $(\tilde{p}, \tilde{q}) \in \mathcal{E}_H$ , while  $D(\tilde{p}, \tilde{q}) \leq 0$  for some  $(\tilde{p}, \tilde{q}) \in \mathcal{E}_H$ , we call system (3.1) having mixed-type equilibria structure.

As an example, we suppose that system (3.1) have hyperbolic structure and apply an  $s$ -stage SRK method  $\mathcal{R}_s$  for its discretization to yield

$$(3.3) \quad \begin{cases} P = p_l e_s + hAF(P, Q), & p_{l+1} = p_l + hb^T F(P, Q), \\ Q = q_l e_s + hAG(P, Q), & q_{l+1} = q_l + hb^T G(P, Q), \end{cases}$$

where  $F(P, Q) = [f(P_1, Q_1), \dots, f(P_s, Q_s)]^T$  and  $G(P, Q) = [g(P_1, Q_1), \dots, g(P_s, Q_s)]^T$  are the internal stage vectors. The corresponding discrete dynamical system for scheme (3.3) is

$$(3.4) \quad \begin{cases} \delta^+ p_l = b^T F(P, Q), \\ \delta^+ q_l = b^T G(P, Q). \end{cases}$$

Clearly, the points in  $\mathcal{E}_H$  are still the equilibrium points (or fixed points) of (3.4). The stability matrix for (3.4) is

$$\mathbf{J}_N = \begin{bmatrix} b^T \partial F / \partial p_l & b^T \partial F / \partial q_l \\ b^T \partial G / \partial p_l & b^T \partial G / \partial q_l \end{bmatrix}.$$

Therefore, in order to preserve the underlying equilibria structure for the numerical scheme, we need to study the matrix structure of  $\mathbf{J}_N(\tilde{p}, \tilde{q})$  with  $(\tilde{p}, \tilde{q}) \in \mathcal{E}_H$ , as what we have done before. Obviously, such arguments apply equally to SPRK methods, and to Hamiltonian systems having the other two kinds of equilibria structures. In the sequel, as an application, we give an example. Consider the following separable 1-d.o.f. Hamiltonian system

$$(3.5) \quad \begin{cases} \dot{p} = \alpha p(1 - p), \\ \dot{q} = \alpha(2p - 1)q, \end{cases}$$

where  $\alpha > 0$ . This problem has been studied in [3], and the solutions  $p(t) \uparrow 1(t \rightarrow +\infty)$  if  $0 < p(t_0) < 1$ , and  $p(t) \downarrow 1(t \rightarrow +\infty)$  if  $p(t_0) > 1$ ; while for any  $q(t_0) > 0$ ,  $q(t) \uparrow +\infty(t \rightarrow +\infty)$  if  $p(t_0) > 1/2$ , and if  $0 < p_0 < 1/2$ ,  $q(t)$  is first monotonically decreasing for  $t < t_0 = (\ln(1 - p(t_0)) - \ln p(t_0)) / \ln \alpha$  and then  $q(t) \uparrow +\infty$  for  $t(> t_0) \rightarrow +\infty$ . It can be seen that  $(0, 0)$  and  $(1, 0)$  are two hyperbolic equilibrium points for (3.5). The stability matrices here are

$$(3.6) \quad \mathbf{J}_S(0, 0) = \begin{bmatrix} \alpha & 0 \\ 0 & -\alpha \end{bmatrix}, \quad \text{and} \quad \mathbf{J}_S(1, 0) = \begin{bmatrix} -\alpha & 0 \\ 0 & \alpha \end{bmatrix}.$$

The symplectic Euler method for (3.5) is read as

$$\begin{cases} p_{l+1} = (1 + z)p_l - zp_l^2, \\ q_{l+1} = q_l + z(2p_l - 1)q_{l+1}, \quad z = \alpha h. \end{cases}$$

or, equivalently,

$$(3.7) \quad \begin{cases} \delta_t^+ p_l = \alpha p_l(1 - p_l), \\ \delta_t^+ q_l = \alpha \frac{(2p_l - 1)q_l}{1 + z - 2zp_l}. \end{cases}$$

We have the following theorem for scheme (3.7) to give a true simulation (see [3])

**Theorem 3.1.** *The sequence  $\{p_l\} \rightarrow 1$  and  $\{q_l\} \rightarrow +\infty$  as  $n \rightarrow +\infty$  iff*

$$(3.8) \quad 0 < z < 1 \quad \text{and} \quad p(t_0) < \frac{1+z}{2z}.$$

If condition (3.8) is destroyed, then it is shown in [3] that spurious solutions or even periodic solutions will be encountered. Through straightforward calculations, the stability matrices of the discrete dynamic (3.7) at its equilibrium points are given by

$$\mathbf{J}_N(0,0) = \begin{bmatrix} \alpha & 0 \\ 0 & -\alpha/(1+z) \end{bmatrix} \quad \text{and} \quad \mathbf{J}_N(1,0) = \begin{bmatrix} -\alpha & 0 \\ 0 & \alpha/(1-z) \end{bmatrix}.$$

In comparison with the stability matrices in (3.6), we see that for scheme (3.7) to preserve the hyperbolic equilibria structure, we need require  $1 - z > 0$ , i.e.,  $0 < z < 1$ . That is, the preservation of equilibria structures only endows the numerical integrator a prerequisite for successful simulations.

For Hamiltonian systems of higher dimensions, the situation will become much more complicated. However, we can make use of the usual linearization techniques for our investigations, which are interesting topics for our future study.

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